# Stochastic mean-field dynamics for fermions in the weak coupling limit

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(Dated: February 1, 2008)

Assuming that the effect of the residual interaction beyond mean-field is weak and has a short memory time, two approximate treatments of correlation in fermionic systems by means of Markovian quantum jump are presented. A simplified scenario for the introduction of fluctuations beyond mean-field is first presented. In this theory, part of the quantum correlations between the residual interaction and the one-body density matrix are neglected and jumps occur between many-body densities formed of pairs of states $D = |\Phi_a\rangle \langle\Phi_b| \,/\, \langle\Phi_b \,|\, \Phi_a\rangle$ where $|\Phi_a\rangle$ and $|\Phi_b\rangle$ are antisymmetrized products of single-particle states. The underlying Stochastic Mean-Field (SMF) theory is discussed and applied to the monopole vibration of a spherical $^{40}$Ca nucleus under the influence of a statistical ensemble of two-body contact interaction. This framework is however too simplistic to account for both fluctuation and dissipation. In the second part of this work, an alternative quantum jump method is obtained without making the approximation on quantum correlations. Restricting to two particles-two holes residual interaction, the evolution of the one-body density matrix of a correlated system is transformed into a Lindblad equation. The associated dissipative dynamics can be simulated by quantum jumps between densities written as $D = |\Phi\rangle \langle\Phi|$ where $|\Phi\rangle$ is a normalized Slater determinant. The associated stochastic Schroedinger equation for single-particle wave-functions is given.

PACS numbers: 24.10.Cn, 24.60.Ky, 21.60.Ka
Keywords: time-dependent Hartree-Fock, stochastic theories, many-body dynamics

arXiv:quant-ph/0509038v2 16 Jan 2006

## I. INTRODUCTION

The description of quantum self-interacting systems with many degrees of freedom is common to many fields of physics, including Bose-Einstein condensates, atomic clusters and nuclear systems. A striking aspect related to this problem is the emergence of well ordered motion at the same time as complexity and chaos [1, 2]. In many situations, the self-consistent mean-field theory provides a suitable framework to describe ordered motions. It also corresponds to one of the most useful method to study the static and dynamical properties of self-interacting systems[3, 4, 5]. However, it often turns out that mean-field reproduces average properties of one-body observables but underestimates dissipative and fluctuating aspects. This can directly be assigned to the absence of two-body effects beyond mean-field. In the nuclear context, it has been proposed to extend mean-field theory by considering that one-body degrees of freedom represents a subsystem which is coupled to more complex internal degrees of freedom. By doing so, the problem of self-interacting system has been mapped to an open quantum system problem. In nuclei, extensive work has been devoted to the formal derivation of dissipative quantum mechanics [6] and/or related stochastic equations for fermions, including Markovian and non-Markovian effects [7, 8, 9, 10, 11, 12, 13, 14]. These approaches have in common that the residual part of the interaction introduces disorder on top of the mean field. These theories end with rather complex transport equations which are hardly applicable in realistic situations [15]. In fact, only recently, the theory proposed in ref. [11] has been applied to small amplitude collective vibrations [16]. Its application to large amplitude motion in non-equilibrated quantum many-body dynamics remains an open issue [15, 17].

During the past decades, large theoretical efforts have been devoted to the development of Monte-Carlo methods to describe the static properties of many-body interacting systems [18]. Recent applications to nuclear physics have shown that stochastic methods can successfully be applied to describe the structure of nuclei [19]. These methods can also be extended to dynamical problems [5] and has been used recently to treat the exact dynamics of interacting bosons [20] or fermions [21] in schematic cases. As underlined in ref. [22], it is highly desirable to provide approximate theory in order to describe dissipation in many-body systems taking advantage of recent advances in Monte-Carlo methods. The present work is an exploratory study devoted to the description of dissipation and fluctuations in dynamical problems using quantum jump techniques. Starting from a perturbative treatment of the residual interaction, two strategies are used to transform the many-body dynamics into a stochastic process. In the first strategy, neglecting part of the quantum correlations, a stochastic theory that may be economical in terms of numerical implementations is obtained. While appropriate to treat fluctuations beyond mean-field, it is however not suitable for dissipation. In the second part of this article, we show that the approximate treatment of quantum correlations can be avoided leading to a more general framework. In that case, the dynamical equation of motion of one-body degrees of freedom can be mapped into a Lindblad equation [23, 24] generally found in the theory of open quantum systems [25]. The

associated jump process is finally discussed.

### A. Generalities on perturbation theory and stochastic mechanics

We consider a many-body fermionic system described by a two-body Hamiltonian $H$. We assume that the mean-field theory already provides a good approximation of its static and dynamical properties. In this case, the N-body wave function can be replaced by an antisymmetrized product of single particle states interacting through an effective self-consistent mean-field, denoted by $H_{MF}$. Let us assume that the system is initially a Slater determinant, denoted by $|\Phi(t)\rangle$ and let us introduce the mean-field propagator $U_{MF}(t',t)$. The great advantage of mean-field theory, is that the propagated many-body state $|\Phi(t')\rangle = U_{MF}(t',t)\,|\Phi(t)\rangle$ remains a Slater determinant and the dynamical evolution of the system reduces to the evolution of its single-particle components. Thus, the many-body density $D$ is approximated by $D \simeq |\Phi(t')\rangle\langle\Phi(t')|$. Accordingly, all the information on the system is contained in the one-body density matrix, denoted by $\rho$, whose matrix elements are defined by $\langle j\,|\rho|\,i\rangle = Tr\left(a_i^+ a_j D\right) \equiv \left\langle a_i^+ a_j\right\rangle$. Mean-field theory does simplify the dynamical description of many-body systems by reducing significantly the number of degrees of freedom to follow in time.

In nuclear physics, mean-field is often adequate to describe average properties of one-body observables but fails to account for fluctuations. At the wave-function level, this corresponds to a deviation of the mean-field trajectory from the exact dynamics [26, 27].

In order to illustrate this effect, we denote by $\delta v_{12}$ the residual two-body interaction defined through $\delta v_{12} = H - H_{MF}$. In the weak coupling regime, this deviation can be treated in perturbation theory and the state at time $t'$ reads [12]

$$|\Psi(t')\rangle \;=\; |\Phi(t')\rangle - \frac{i}{\hbar}\int \delta v_{12}(s)\,|\Phi(s)\rangle\,ds - \frac{1}{2\hbar^2}T\left(\int\int \delta v_{12}(s')\delta v_{12}(s)ds'ds\,|\Phi(s)\rangle\right). \tag{1}$$

$\delta v_{12}(s)$ corresponds to the residual interaction written in the interaction picture, $\delta v_{12}(s) = U_{MF}^+(s,t)\delta v_{12}(t)U_{MF}(s,t)$. While at the mean-field level, $|\Psi(t')\rangle$ is replaced by $|\Phi(t')\rangle$, due to the accumulated effect of $\delta v_{12}$ in time, it is expected that the exact state becomes a more and more complex superposition of a large number of Slater determinants. Accordingly, the information on the system cannot be reduced anymore to the knowledge of the one-body density matrix only and higher order correlations must be accounted for. A natural extension of mean-field theory is to enlarge the number of degrees of freedom considered. This is done for instance in the Time-Dependent Density Matrix theory (TDDM) where both the one-body density matrix and the two-body correlation operator are followed in time [28]. These theories are however rarely applied due to the large number of degrees of freedom to consider [29].

An alternative way to account for correlations beyond mean-field is to use stochastic methods. Several strategies have been proposed to introduce noise on top of the mean-field, either based on statistical ensemble of one-body densities [7, 10, 11], random two-body interactions or phase shift [8, 9], or directly from Fermi golden rule [12, 13, 14]. The goal in all cases, is to simulate the dynamics of correlated system by averaging over an ensemble of mean-field trajectories. The great advantage in that case, is that the number of degrees of freedom to follow along each path is not increased compared to standard mean-field. However, these theories are rather complex and methods for numerical implementations are still missing.

The aim of the present work is to discuss again the possibility to replace correlated dynamics by quantum jumps in the Hilbert space of Slater determinants. We use equation (1) as a starting point and we restrict the discussion to the Markovian limit. In order to illustrate this hypothesis, we follow ref. [8, 9]. We assume that the residual interaction induces random transitions treated as a statistical ensemble of two-body interactions acting on top of the mean-field. Eq. (1) is then replaced by a set of evolutions with the same initial state and mean-field but with different residual interactions. We assume that the two-body operator has a gaussian distribution with a mean value $\overline{\delta v_{12}} = 0$ and a second moment denoted by $\overline{\delta v_{12}^2}$. Here, the average is taken over different values of $\delta v_{12}$. In nuclear systems, the residual interaction is expected to induce transitions on a shorter time scale (called correlation time and denoted by $\tau$) than the time associated to the mean field evolution (denoted by $\tau_{rel}$)[17, 30]. $\tau$ is related to the average autocorrelation function $\overline{\delta v_{12}(s')\delta v_{12}(s)}$ which is approximated by [8, 9]

$$\overline{\delta v_{12}(s')\delta v_{12}(s)} \propto \overline{\delta v_{12}^2(s)}e^{-(s-s')^2/2\tau^2}. \tag{2}$$

Using this approximation, we consider a time-scale $\Delta t$ much larger than the time $\tau$ but smaller than $\tau_{rel}$. In the following, this limit will be called "Markovian" or "short memory time" approximation.

Using approximation (2), we consider in the following two limits for which the wave function evolution as given by (1) can be replaced by quantum jumps between Slater determinants. The first case is a simplified scenario where part

of quantum correlations between $\delta v_{12}$ and $\rho$ are neglected along the path. In this case, it is shown that the evolution can be formulated in terms of quantum jumps between many-body densities formed of pairs of Slater determinants. In a second part, we show that the perturbative dynamics can still be transformed into a quantum jump process even if quantal correlations are not neglected. In both cases, all equations necessary for applications are given explicitly.

## II. FLUCTUATIONS BEYOND MEAN-FIELD IN A SIMPLIFIED STOCHASTIC SCENARIO

Let us first consider the perturbative evolution of an initial Slater determinant. Assuming equation (2) and the short memory time approximation, the mean-field does not change over $\Delta t$. Then, the average evolution of the state, denoted by $\overline{\Delta\left|\Psi\right\rangle} = \overline{\left|\Psi(t+\Delta t)\right\rangle} - \left|\Phi(t)\right\rangle$, reduces to

$$\overline{\Delta\left|\Psi\right\rangle} = \frac{\Delta t}{i\hbar} H_{MF}\left|\Phi(t)\right\rangle - \frac{\tau\Delta t}{2\hbar^2}\,\overline{\delta v_{12}^2}\left|\Phi(t)\right\rangle. \tag{3}$$

This expression can also be regarded as an average over Markovian stochastic processes in many-body wave-functions space. To give a deeper insight we define the ensemble of antisymmetrized two-body residual interactions as

$$\delta v_{12}(\sigma) = \frac{1}{4}\sum_{\alpha\beta\gamma\delta} a_\alpha^+ a_\beta^+ \left\langle\alpha\beta\left|\delta v_{12}(\sigma)\right|\delta\gamma\right\rangle a_\gamma a_\delta. \tag{4}$$

Here, $\sigma \equiv \{\sigma_i\}_{i=1,N}$ where all components are stochastic variables sampled according to gaussian probabilities with mean zero and $\overline{{\sigma_i}^2} = 1$. The number $N$ of stochastic components defines the complexity of the process. The definition (4) includes the force proposed in ref. [9]. Eq. (3) can be interpreted as the average over the quantum diffusion

$$\Delta\left|\Psi\right\rangle = \left\{\frac{\Delta t}{i\hbar}H_{MF} + \Delta B\delta v_{12} + \frac{1}{2}\left(\Delta B\delta v_{12}\right)^2\right\}\left|\Phi(t)\right\rangle, \tag{5}$$

where $\Delta B = i\sqrt{\tau\Delta t}/\hbar$. In the following, we will consider last expression as a differential stochastic equation in Hilbert space [25, 31]. We use the notation $dB$ instead of $\Delta B$ and use the Ito rules of stochastic calculus [32]. Due to the two-body nature of $\delta v_{12}$, eq. (5) induces complex reorganization of single-particle degrees of freedom. After the jump, the state is not a priori a single Slater determinant. For applications, it is highly desirable to preserve the simple initial form of the state along the stochastic path. This could be achieved by invoking additional approximations described below. Following ref. [20, 21, 22], we consider an initial density

$$D = \frac{\left|\Phi_a\right\rangle\left\langle\Phi_b\right|}{\left\langle\Phi_b\mid\Phi_a\right\rangle}, \tag{6}$$

where $\left|\Phi_a\right\rangle = \mathcal{A}\left(\Pi_i\left|\alpha_i\right\rangle\right)$ and $\left|\Phi_b\right\rangle = \mathcal{A}\left(\Pi_i\left|\beta_i\right\rangle\right)$ are two non-orthogonal Slater determinants formed of products of single particle wave packets denoted respectively by $\left|\alpha_i\right\rangle$ and $\left|\beta_i\right\rangle$. The notation $\mathcal{A}(.)$ corresponds to the antisymmetrized product. We assume that both states follow the diffusion process described by eq. (5) but with two independent sets of gaussian stochastic variables, denoted respectively by $\sigma_{\mathbf{a}}$ and $\sigma_{\mathbf{b}}$. This case will be referred in the following as the "uncorrelated noise". The use of different sets of stochastic variables is at variance with standard quantum Monte-Carlo procedures that simulate density evolution given by Lindblad equations[25]. However, this assumption has been shown to be crucial in order to describe the exact dynamics of interacting systems with stochastic methods [20, 21].

### A. Approximate stochastic mechanics in one-body density matrix space

To approximate the diffusion process, we first focus on single-particle degrees of freedom. Under the approximation

$$\begin{aligned}\left\langle a_i^+ a_j \delta v_{12}^2\right\rangle \quad &\simeq \left\langle a_i^+ a_j\right\rangle\left\langle\delta v_{12}^2\right\rangle + 2\left\langle a_i^+ a_j\delta v_{12}\right\rangle\left\langle\delta v_{12}\right\rangle \\ &\quad -2\left\langle a_i^+ a_j\right\rangle\left\langle\delta v_{12}\right\rangle^2,\end{aligned} \tag{7}$$

the one-body density evolution (eq. (5)) reduces to

$$\begin{aligned} d\left\langle a_i^+ a_j\right\rangle \;&\simeq\; \frac{dt}{i\hbar}\left\langle\left[a_i^+ a_j, H_{MF}\right]\right\rangle \\ &+\; dB_a\left(\left\langle a_i^+ a_j\delta v_{12}\right\rangle - \left\langle a_i^+ a_j\right\rangle\left\langle\delta v_{12}\right\rangle\right) \\ &+\; dB_b^*\left(\left\langle\delta v_{12} a_i^+ a_j\right\rangle - \left\langle a_i^+ a_j\right\rangle\left\langle\delta v_{12}\right\rangle\right). \end{aligned} \tag{8}$$

It is interesting to notice that, although we consider a second-order perturbation theory for the residual interaction, the second order term exactly cancels out when approximation (7) is used. Eq. (7) corresponds to a gaussian approximation for quantal fluctuations. Therefore, eq. (8) provides the stochastic equation of motion of one-body degrees of freedom associated to eq. (5) when neglecting part of the quantal fluctuations. The corresponding stochastic evolution of $\rho$ reads

$$\begin{aligned} d\rho = \frac{dt}{i\hbar}\left[h_{MF},\rho\right] \; &+ \; dB_a(1-\rho)U(\rho,\sigma_{\mathbf{a}})\rho \\ &+ \; dB_b^*\rho U'(\rho,\sigma_{\mathbf{b}})(1-\rho), \end{aligned} \tag{9}$$

where $h_{MF}$ denotes the matrix elements associated to the mean-field Hamiltonian while $U(\rho,\sigma_{\mathbf{a}}) = Tr_2(\delta v_{12}(\sigma_{\mathbf{a}})\rho_2)$ and $U'(\rho,\sigma_{\mathbf{b}}) = Tr_2(\rho_2\delta v_{12}(\sigma_{\mathbf{b}}))$.

The stochastic one-body evolution given by eq. (9) contains also part of the information on correlations. Indeed, an approximate evolution of the two-body density, whose matrix elements are $\left\langle a_i^+ a_j^+ a_l a_k\right\rangle = \langle kl\left|\rho_{12}\right|ij\rangle$ can be obtained through approximations similar to eq. (7) but preserving the symmetry of the two-body density:

$$\begin{aligned} < a_i^+ a_j^+ a_l a_k v_{12} > \; &\simeq \; < a_i^+ a_j^+ a_l a_k >< v_{12} > + \left(< a_i^+ a_k v_{12} >< a_j^+ a_l > - < a_i^+ a_l v_{12} >< a_j^+ a_k >\right) \\ &+ \; \left(< a_i^+ a_k >< a_j^+ a_l v_{12} > - < a_i^+ a_l >< a_j^+ a_k v_{12} >\right) \\ &- \; 2\left(< a_i^+ a_k >< a_j^+ a_l > - < a_i^+ a_l >< a_j^+ a_k >\right) < v_{12} > \end{aligned} \tag{10}$$

and

$$\begin{aligned} < a_i^+ a_j^+ a_l a_k v_{12} v_{12} > \; &\simeq \; < a_i^+ a_j^+ a_l a_k >< v_{12}^2 > + 2\left(< a_i^+ a_k v_{12} >< a_j^+ a_l v_{12} > - < a_i^+ a_l v_{12} >< a_j^+ a_k v_{12} >\right) \\ &- \; 2\left(< a_i^+ a_k >< a_j^+ a_l > - < a_i^+ a_l >< a_j^+ a_k >\right) < v_{12} >^2 . \end{aligned} \tag{11}$$

Combining with Ito rules, the evolution of $\rho_{12}$ reduces to

$$d < a_i^+ a_j^+ a_l a_k > \simeq d(\rho_{ki}\rho_{lj} - \rho_{kj}\rho_{li}) \tag{12}$$

indicating that the two-body evolution can be deduced from the stochastic evolution of $\rho$. Although eq. (12) is similar to the mean-field case, it contains correlations beyond mean-field. A similar situation occurs in the exact reformulation of self-interacting fermions with quantum jumps [22].

In summary, the jump process described by eq. (5) for both state vectors entering in $D$ can be approximated by the jump process in one-body space given by eq. (9) if part of the quantal fluctuations are neglected. The advantage of this approximation is that expression (6) for $D$ is preserved along the stochastic path. In this work, we restrict ourself to this limit and eq. (9) will be referred to the incoherent Stochastic Mean-Field (SMF) dynamics. The properties of this diffusion process are described below.

We consider that the single-particle states of $|\Phi_a\rangle$ and $|\Phi_b\rangle$ initially verify

$$\langle\beta_j \mid \alpha_i\rangle = \delta_{ij}. \tag{13}$$

Eq. (9) can be simulated by quantum jumps for single-particle states given by

$$\begin{cases} |d\alpha_i\rangle \; = \; \left[\frac{dt}{i\hbar}h_{MF}(\rho) + dB_a(1-\rho)U(\rho,\sigma_{\mathbf{a}})\right]|\alpha_i\rangle \\ \langle d\beta_j| \; = \; \langle\beta_j|\left[-\frac{dt}{i\hbar}h_{MF}(\rho) + dB_b^*U'(\rho,\sigma_{\mathbf{b}})(1-\rho)\right]. \end{cases} \tag{14}$$

The latter quantum diffusion process has several attractive aspects. First, it can be easily verified that eq. (13) is preserved along the stochastic path. Thus, the one-body density reads at all time $\rho = \sum_i |\alpha_i\rangle\langle\beta_i|$. Consequently, the trace of the density is constant along the path: $Tr(dD) = Tr(d\rho) = 0$. In addition, $\rho$ remains a projector, i.e. $\rho^2 = \rho$ at all time. Finally, the total entropy $S = -k_B Tr(D\ln D)$ is constant along the path. Indeed, since the density is given by eq. (6), $S(D)$ identifies with the one-particle entropy $S(\rho)$. Using equation (9) and Ito rules, we obtain $\overline{dS(\rho)} = 0$. Despite a constant entropy, the SMF induces correlations beyond mean-field. Indeed, starting from an initial two-body density $\rho_{12} = \mathcal{A}(\rho_1\rho_2)$, after one time step, the average evolutions of the one- and two-body density matrices read

$$\begin{cases} \overline{d\rho} \; = \; \frac{dt}{i\hbar}\left[h_{MF},\rho\right] \\ \overline{d\rho_{12}} \; = \; \frac{dt}{i\hbar}\left[h_{MF}(1) + h_{MF}(2),\rho_{12}\right] + dC_{12}. \end{cases} \tag{15}$$

The labels "1" and "2" refer to the particle on which the operator is acting [33]. $dC_{12}$ corresponds to correlations beyond mean-field associated to the stochastic one-body evolution given by eq. (9). It reads

$$dC_{12} = -\frac{\tau dt}{\hbar^2} \quad \Big\{(1-\rho_1)(1-\rho_2)\overline{U_1(\sigma_\mathbf{a})U_2(\sigma_\mathbf{a})}\rho_{12} + \rho_{12}\overline{U_1'(\sigma_\mathbf{b})U_2'(\sigma_\mathbf{b})}(1-\rho_1)(1-\rho_2)\Big\}, \tag{16}$$

where the density dependence are omitted in $U$ and $U'$. Eq. (16) clearly indicates that $dC_{12}$ is a second order term in perturbation. Note that it has a similar form as the second moment of the initial stochastic correlation used in ref. [11].

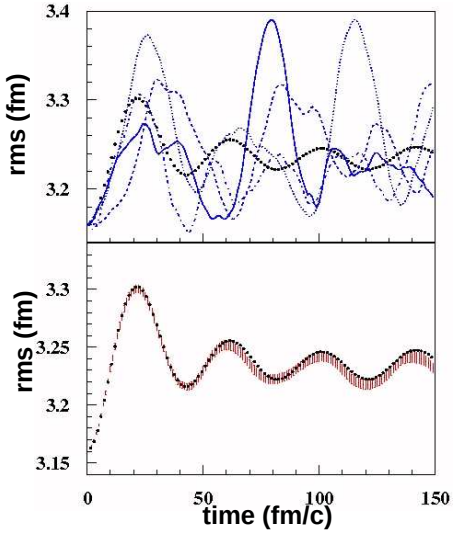


FIG. 1: Top: Evolution of the root mean square radius (rms) as a function of time. Black circles correspond to the standard TDHF evolution while different lines correspond to different stochastic paths. Bottom: Error bars correspond to the rms evolution obtained by averaging over different paths while black circles correspond to the TDHF case. The stochastic simulation is performed for $g_0 = 500$ MeV/fm. The average is taken over 200 trajectories. The width of the error bars correspond to the statistical fluctuations of the rms.

### B. Illustration of application

To illustrate the SMF theory, we consider the monopolar vibration of a $^{40}$Ca nucleus. The system is initially prepared in a pure state $D = |\Phi\rangle\langle\Phi|$, where $|\Phi\rangle$ is a Slater determinant solution of a constrained Hartree-Fock (CHF) equation. The CHF equation is solved assuming spherical symmetry and spin and isospin saturation. The Skyrme interaction of ref. [34] is used in the mean-field. We assume in addition to the self-consistent mean-field, a monopolar constraint $\lambda r^2$ with $\lambda = 0.25$ MeV.fm$^{-2}$ at $t < 0$ fm/c [35]. At $t = 0$ fm/c, the constraint is relaxed and two dynamical calculations are considered. The first one corresponds to the time-dependent Hartree-Fock (TDHF) evolution. In the second case, the SMF evolution described by eq. (9) is performed with a statistical ensemble of contact interactions defined by one stochastic variable, i.e. $\delta v_{12}(\sigma) = \sigma v_{res}$ where $v_{res}$ is a contact interaction. In this case, $U(\sigma, r)$ takes the form $U(\sigma, r) = \sigma g_0 \rho(r)$, where $g_0$ is a parameter measuring the strength of the perturbation. In both cases, evolutions are solved assuming spherical symmetry.

The evolution of the root mean square radius (rms) obtained with TDHF is presented in figure 1 (filled circles). The different lines displayed on the top part of figure 1 correspond to the evolution of the rms along several stochastic paths obtained with $g_0 = 500$ MeV/fm and a collision time $\tau = 0.01$ fm. In each case, the stochastic evolution differs significantly from the mean-field prediction. Bottom part of figure 1 shows a comparison between the TDHF evolution and the evolution of the rms obtained by averaging over the different stochastic trajectories. Interestingly enough, the average evolution identifies with the TDHF evolution. This example illustrates a special situation where the mean-field dynamics can be recovered from complex trajectories in many-body space [36]. However, significant fluctuations around the mean TDHF trajectories are observed. This is illustrated in figure 2 where the quantity $\Delta_r = \sqrt{\overline{\langle r^2\rangle^2} - \overline{\langle r^2\rangle}^2}$ is displayed as a function of time for different values of $g_0$ and $\lambda$. We also computed as a reference

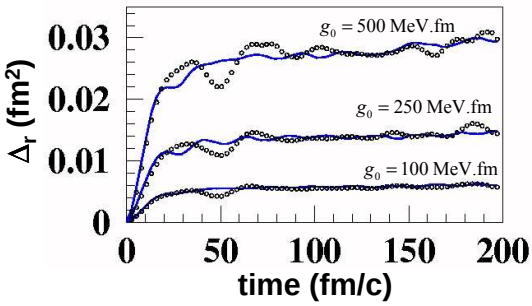


FIG. 2: Evolution of the dispersion of the rms as a function of time for different values of $g_0$. The different curves from bottom to top corresponds respectively to $g_0 = 100$, 250 and 500 MeV.fm. Solid lines and open circles correspond respectively to an initial constraint $\lambda = 0$ MeV.fm$^{-2}$ and $\lambda = 0.25$ MeV.fm$^{-2}$.

the mean-field width $\sigma_{MF}$, corresponding to the quantal fluctuations of $r^2$ estimated in the mean-field approximation, leading to $\sigma_{MF} = 6.3fm^2$. As we do expect in the weak coupling approximation, the additional fluctuations $\Delta_r$ induced by the stochastic term are much smaller than $\sigma_{MF}$. It turns out that the dispersion is properly parametrized by the formula $\Delta_r = \Delta_0(1 - e^{-\Gamma_0 t})$ where $\Delta_0$ is proportional to $g_0$ while $\Gamma_0$ is independent of it. Therefore, while the average evolution of the rms collective variables is not affected by the stochastic process, fluctuations around the mean value increases and saturates as we do expect in Brownian motion. Interestingly enough, the behavior observed here is very similar to the description of a quantum oscillator [37] with Nelson stochastic mechanics [38] replacing $(\hbar/m)^{1/2}$ by $g_0$. Assuming a single collective state and using similar techniques as in ref. [37], analytical expression can be obtained for $\Delta_r$ where $\Delta_0$ is indeed proportional to $g_0$ while $\Gamma_0$ depends only on the oscillator frequency. Note however that a complete understanding of the Brownian process presented here pass through the linearization of eq. (9) as in ref. [17].

### C. Critical discussion

In this section, it has been shown that the presented SMF theory can be applied to account for fluctuations beyond mean-field. The above example can only serve as an illustration due to the very schematic residual interaction used and to the very small time $\tau$ (see estimation in ref. [39, 40]). Besides the simplicity of the force, it is important to note that the above theory only gives a partial answer to the simulation of correlations beyond mean-field for realistic nuclear systems. Indeed, as clearly seen in figure (1), while fluctuations of one-body observables are increased, the average evolution of the rms identifies with the TDHF case. Therefore, no additional damping is observed in SMF in opposite to what is obtained in extended Time-Dependent Hartree-Fock (extended TDHF) [17]. Indeed, dissipative aspects present in the memory kernel of extended TDHF are not included in the present framework. A careful analysis demonstrates that the absence of a collision term could be assigned to the approximations made on quantal fluctuations (equation (7), (10) and (11)).

Under these approximations, it is however possible to show that a fermionic system submitted to a statistical ensemble of residual interactions $\delta v_{12}$ can be treated by a jump process related to its mean-field (equation (9)). The form of the noise is a second critical aspect for nuclear physics. In fact, it is expected that the residual interaction is dominated by the two-particle two-holes (2p-2h) channels. Due to the mean-field nature of the noise in eq. (9), these components cancel out in the stochastic part. Therefore, while the above SMF can be of great interest, some important aspects for nuclear physics are missing. In the next section, we discuss the possibility to use quantum jump process in one-body space in a more general framework.

## III. STOCHASTIC MECHANICS WITH DISSIPATION

In order to generalize the stochastic method described previously, we consider directly the evolution of the many-body density $D$ associated to eq. (1). Using the short memory time approximation for $\delta v_{12}$, the evolution of $D$ can be recast as

$$\Delta D = \frac{\Delta t}{i\hbar}[H_{MF}, D] - \frac{\tau \Delta t}{2\hbar^2}\overline{[\delta v_{12}, [\delta v_{12}, D]]}. \tag{17}$$

In the previous section, the term $\overline{\delta v_{12} D \delta v_{12}}$ has been neglected due to the fact that the average evolution of wave-functions were directly considered. Due to this approximation, it was possible to have uncorrelated noise for $|\Phi_a\rangle$ and $\langle\Phi_b|$. Here, this contribution is not neglected. As a consequence, the uncorrelated noise assumption is not possible anymore.

The one-body density matrix equation of motion associated to (17) is given by

$$\frac{d\rho}{dt} = \frac{1}{i\hbar}\left[h_{MF}(\rho), \rho\right] - \frac{g}{2}\mathcal{D}(\rho), \tag{18}$$

where $g$ is a real constant, $g = \tau/\hbar^2$. $\mathcal{D}(\rho)$, called "dissipator" hereafter, corresponds to the average effect of the residual interaction and reads

$$\langle j\left|\mathcal{D}\right|i\rangle = \overline{\left\langle\left[\left[a_i^+ a_j, \delta v_{12}\right], \delta v_{12}\right]\right\rangle}. \tag{19}$$

We assume that the system is initially in a pure state described by a Slater determinant $|\Phi(t)\rangle$ formed of $N$ orthonormal single particle states denoted by $|\alpha\rangle$. The associated initial one-body density matrix reads $\rho = \sum_\alpha |\alpha\rangle\langle\alpha|$. Having in mind the nuclear many-body problem, we assume that only 2p-2h components of $\delta v_{12}$ are not equal to zero. Completing the hole states by a set of particle states, denoted by $|\tilde{\alpha}\rangle$, we have:

$$\delta v_{12}(t) = \frac{1}{4}\sum_{\tilde{\alpha}\tilde{\beta}\alpha\beta} a_{\tilde{\alpha}}^+ a_{\tilde{\beta}}^+ \left\langle\tilde{\alpha}\tilde{\beta}\left|v_{12}(t)\right|\alpha\beta\right\rangle a_\alpha a_\beta. \tag{20}$$

$\mathcal{D}$ can then be recast as

$$\mathcal{D}(\rho) = Tr_2\left[v_{12}, F_{12}\right], \tag{21}$$

where $F_{12}$ is equal to

$$\begin{aligned} F_{12} &= \frac{1}{2}\left\{\left(1-\rho_1\right)\left(1-\rho_2\right)v_{12}\rho_1\rho_2\right. \\ &\quad \left. - \rho_1\rho_2 v_{12}\left(1-\rho_1\right)\left(1-\rho_2\right)\right\}. \end{aligned} \tag{22}$$

Expression (21) takes a form similar to the collision term generally obtained in extended TDHF [17]. The dissipator $\mathcal{D}(\rho)$ can be further transformed. Indeed, $\delta v_{12}$ given by eq. (20) can always be decomposed as (see for instance [41])

$$\delta v_{12} = -\frac{1}{4}\sum_n \lambda_n \mathcal{O}_n^2, \tag{23}$$

where $\lambda_n$ are real and the $\mathcal{O}_n$ correspond to a set of commuting Hermitian one-body operators written as $\mathcal{O}_n = \sum_{\tilde{\alpha}\alpha}\langle\tilde{\alpha}\left|O_n\right|\alpha\rangle a_{\tilde{\alpha}}^+ a_\alpha$. Reporting in eq. (21), $\mathcal{D}(\rho)$ can be recast as

$$\mathcal{D}(\rho) = \sum_{mn}\Gamma_{mn}\left[O_n O_m\rho + \rho O_n O_m - 2O_m\rho O_n\right]. \tag{24}$$

The coefficient $\Gamma_{mn}$ are given by

$$\Gamma_{mn} = \frac{1}{2}\lambda_m\lambda_n Tr(O_m(1-\rho)O_n\rho). \tag{25}$$

We recognize in this expression, the quantum covariance between the operator $\mathcal{O}_n$ and $\mathcal{O}_m$ , i.e. $Tr(O_m(1-\rho)O_n\rho) = \langle\mathcal{O}_m\mathcal{O}_n\rangle - \langle\mathcal{O}_m\rangle\langle\mathcal{O}_n\rangle$. Expression (24) has the form of the dissipator appearing usually in the Lindblad equation[25]. Therefore, we have shown that the evolution of one-body degrees of freedom associated to equation (17) identifies with a Markovian quantum master equation generally obtained in quantum open systems. A large amount of work is devoted to the simulation of such master equation by quantum jump methods (see for instance [25, 42, 43, 44, 45]) and one can take advantage of the most recent advances in this field. This aspect has however rarely been discussed in the context of self-interacting system. In the following, the associated diffusion process is precised and we show that it indeed corresponds to jumps between Slater determinants. The stochastic Schroedinger equation for single-particle wave-function is finally given.

### A. Explicit form of the stochastic process

Following ref. [25], we introduce the Hermitian positive matrix $\Gamma$ with components $\Gamma_{mn}$. An economical method to introduce quantum jump process [25] is to use the unitary transformation $u$ that diagonalizes $\Gamma$, i.e. $\Gamma = u^{-1}\gamma u$, where $\gamma$ is the diagonal matrix of the eigenvalues of $\Gamma$. New operators $A_k$ can be defined by the transformation $A_k = \sum_n u_{kn}^{-1} O_n$. The dissipator is then recast as

$$\mathcal{D}(\rho) = \sum_k \gamma_k \left[ A_k^2 \rho + \rho A_k^2 - 2 A_k \rho A_k \right]. \tag{26}$$

The last equation can be simulated using the average over the stochastic mean-field dynamics:

$$d\rho \;=\; \frac{dt}{i\hbar}\left[h_{MF}(\rho), \rho\right] - g\frac{dt}{2}\mathcal{D}(\rho) + db_{sto}, \tag{27}$$

where $db_{sto}$ is a stochastic one-body operator which, using Ito rules [32], reads

$$db_{sto} \;=\; \sum_k \left\{ dW_k (1-\rho) A_k \rho + dW_k^* \rho A_k (1-\rho) \right\}. \tag{28}$$

Here $dW_k$ denotes stochastic variables given by $dW_k = -i d\xi_k \sqrt{g\gamma_k}$, where $d\xi_k$ corresponds to a set of real gaussian stochastic variables with mean zero and $d\xi_k d\xi_{k'} = \delta_{kk'} dt$.

### B. Nature of the stochastic process in Hilbert space

It is worth noticing that the proposed dissipative equation and its stochastic counterpart are only well defined if the density is initially prepared as a pure Slater-determinant state. We now turn to the essential properties of equation (27). First, it preserves the number of particles $Tr(d\rho) = 0$. In addition, if initially $\rho^2 = \rho$, then

$$d\rho d\rho - g\frac{dt}{2}\left[\rho\mathcal{D}(\rho) + \mathcal{D}(\rho)\rho\right] = -g\frac{dt}{2}\mathcal{D}(\rho) \tag{29}$$

which is obtained using Ito stochastic rules and retaining only terms linear in $dt$. The last expression demonstrates that $(\rho + d\rho)^2 = \rho + d\rho$. Thus, $\rho$ remains a projector along the stochastic path. As a consequence, the pure state nature of the many-body density matrix is preserved along the stochastic path, i.e. $D = |\Phi(t)\rangle \langle\Phi(t)|$ where $|\Phi\rangle$ is a normalized Slater determinant at all time. The associated stochastic Schroedinger equation for single-particle states reads

$$d\,|\alpha\rangle = \left\{ \frac{dt}{i\hbar} h_{MF}(\rho) + \sum_k dW_k (1-\rho) A_k - g\frac{dt}{2}\sum_k \gamma_k \left[ A_k^2 \rho + \rho A_k \rho A_k - 2 A_k \rho A_k \right] \right\} |\alpha\rangle\,. \tag{30}$$

This last expression can be directly used for practical applications.

In this section, assuming that the residual interaction can be written in terms of $2p-2h$ components, we have shown that the dissipative dynamics of one-body degrees of freedom can be simulated by quantum jumps. The stochastic method differs significantly from the simplified scenario considered in previous section. First, the above theory does not require to introduce generalized many-body density matrix formed of two Slater determinants since $D = |\Phi(t)\rangle \langle\Phi(t)|$ along each path. As a counterpart, the numerical effort required to treat the new SMF which includes dissipative aspects is significantly increased. Indeed, in section II B, we have shown that fluctuations can be introduced using simplified residual interaction and a limited number of noise terms. In the new SMF, the numerical effort is directly proportional to the number of one-body operators entering in eq. (23). This situation is similar to stochastic methods used in nuclear structure studies [19]. In that case, large numerical effort is required. For instance, if we assume that a physical system is described in a mesh, then the number of noise terms is is a priori as large as the number of mesh points. The numerical implementation of the quantum jump process in its full complexity is expected to be still difficult with present computers capacities. Therefore, specific numerical techniques as well as truncation procedures should be developed in order to implement the method in many-body dissipative dynamics.

## IV. CONCLUSION

In this work, we have presented a discussion on the possibility to replace the dynamics of interacting fermions by quantum jumps. Assuming a weak coupling approximation and a short memory time for the residual interaction, two scenarios have been considered. Focusing on one-body degrees of freedom, two different approximations lead to equations of motions for the one-body density matrix that can be treated by quantum jumps between Slater determinants.

In the first stochastic mean-field process, part of the quantal correlations between $\rho$ and $\delta v_{12}$ are neglected along the path. The SMF is illustrated in the monopolar vibration of a calcium nucleus. In this case, while expectation values of one-body observables are unchanged, fluctuations are increased compared to mean-field. In the presented application, the residual interaction is rather simple. However, more complex statistical ensembles can be used like two-body random interactions. This method suffers from the absence of dissipative effects and appears to be too simplified for the nuclear many-body problem.

In the second part of this work, we show that the dynamics of correlated systems can be described by a quantum jump process even if no approximation on the quantal correlations are made. Restricting to 2p-2h residual interactions, a guideline is given for transforming the evolution of the one-body density matrix evolution into a Lindblad equation. The stochastic process corresponds to quantum jumps between pure state densities $D = |\Phi\rangle \langle\Phi|$ where $|\Phi\rangle$ is a Slater determinant. The associated stochastic equation of motion for single-particle wave-functions is given.

Finally, we would like to mention that the presented framework does not account for non-Markovian effects. It has however been shown in ref. [15] that the memory effect might be important in the nuclear context. Promising work are actually devoted to incorporate non-Markovian effects in quantum Monte-Carlo methods [46, 47, 48, 49].

**ACKNOWLEDGMENTS**

The author is grateful to Thomas Duguet, Dominique Durand and Cedric Simenel for the careful reading of the manuscript and to Olivier Juillet for discussions during this work.

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